

Phosphonothioic acid, ethyl-, O-ethyl S-phenyl ester

Other names:	O-Ethyl S-phenyl ethanephosphonothioate O-Ethyl S-phenyl ethylphosphonothioate O-Ethyl S-phenyl ethylphosphonothiolate Fonofos oxon Dyfonate O-analog
Inchi:	InChI=1S/C10H15O2PS/c1-3-12-13(11,4-2)14-10-8-6-5-7-9-10/h5-9H,3-4H2,1-2H3
InchiKey:	KKVDUJRKQVHKBU-UHFFFAOYSA-N
Formula:	C10H15O2PS
SMILES:	CCOP(=O)(CC)Sc1ccccc1
Mol. weight [g/mol]:	230.26
CAS:	944-21-8

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.83		Crippen Method
logp	4.028		Crippen Method
mcvol	176.550	ml/mol	McGowan Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C944218&Units=SI

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume

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